
Module 2: Estimating emissions and exposures: Case studies from the PMN process

David Allen, Department of Chemical Engineering
University of Texas at Austin

Nhan Nguyen, U.S. Environmental Protection Agency

Module 2: Estimating emissions and exposures: Case studies from the PMN process

- Educational goals and topics covered in the module
- Potential uses of the module in chemical engineering courses
- Student handouts
- Instructor materials and textbook
- Software
- Case studies

Module 2: Educational goals and topics covered in the module

Students will:

- become familiar with the PreManufacture Notice (PMN) process
- be able to estimate emissions and exposures, based on limited process data
- be able to identify potential sources of emissions in flowsheets
- be aware of the limitations of emission and exposure estimation methods

Module 2: Educational goals and topics covered in the module (cont'd)

Topics covered:

- PMN process
- Emission estimation methods
- Exposure estimation methods
- Chemical Ranking schemes used in the PMN process
- Relative risk assessments

Module 2: Potential uses of the module in chemical engineering courses

- Design course: Use as a preliminary screen of chemical products and raw materials; use as a preliminary flowsheet assessment tool
- Courses on Industrial chemistry, polymers, electronic materials: Module on environmental impacts

Module 2: Student handouts

- Chapter 6 from textbook
- Class lecture notes: edited from chapter 6 and designed so that instructor writes in key concepts and calculations during the lecture
- Problem 1: PMN case study of a fragrance

Module 2: Instructor materials

- Completed class lecture notes: edited from chapter 6; contains material that the instructor writes into the notes during the lecture
- Problem 1: PMN case study of a fragrance

Module 2: Software

CHEMSTEER, CRSS, STP and ECOSAR
collection of software programs - Topics
covered:

- Emission estimation
- Exposure estimation
- Toxicity

CHEMSTEER/CRSS/STP/ECOSAR: Software Demonstration

Module 2, Case study 1: PMN case study of a polymer product

A company wishes to use

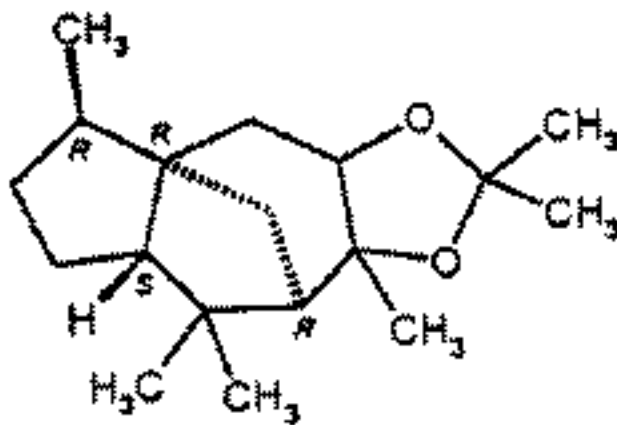
4H-4a,9-Methanoazuleno[5,6-d]-1,3-
diazole,octahydro-2,2,5,8,8,9a-
hexamethyl-(4aR,5R,7aS,9R)

It will be blended with other products and will be used at a rate of a few hundred kg/yr. It is used as a fragrance in cleaners, room fresheners, and other products. It will be processed as a 10% solution in dipropylene glycol

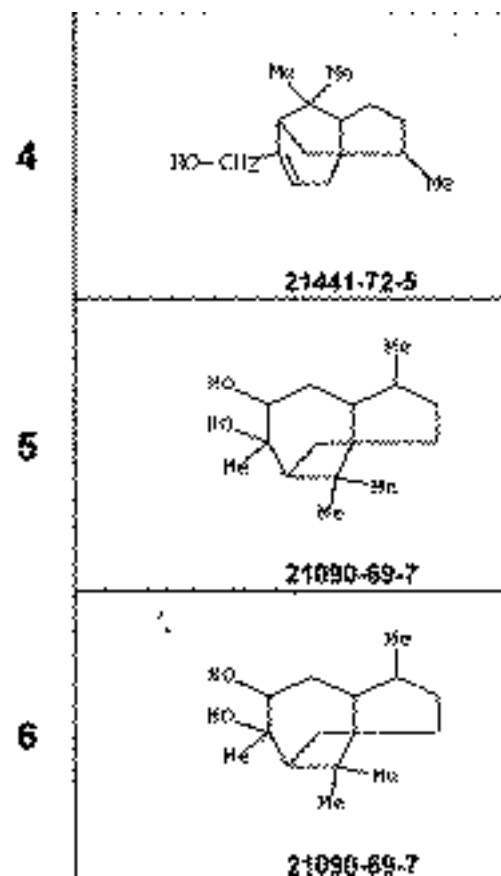
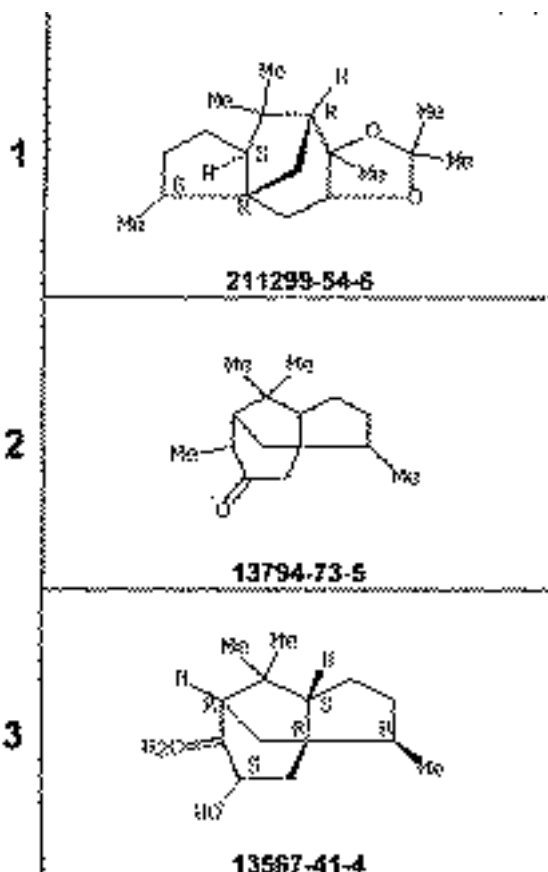
Case study 1

- Review structure
- Review flowsheet
- Identify and estimate relevant properties
- Estimate emissions
- Estimate exposures
- Assess relative risk

Chemical Structures



Chemical Structures



Flowsheet

- Sample from packaging container on receipt
- Pour product into container and transfer to mixing vessel
- Mix with other fragrance products
- Repackage

Estimate emissions, exposures and potential risks

- **Environmental risks** Assume 96 kg/yr of releases through wastewater and 550 kg/yr through wastewater releases due to industrial use; other releases less than trigger amounts; estimate stream concentrations, drinking water concentrations and ingestion due to fish consumption

- **Consumer risks**

1. Dermal contact in soaps; estimate events over a 70 year lifetime; estimate exposure based on skin area
2. Inhalation through use in room freshener; calculate room exchange rates and inhalation rate